

Excitation Spectra of Correlated Lattice Bosons in a Confining Trap

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We consider ultracold bosonic atoms in an optical lattice with an external trapping potential. To study the excitation energies of the resulting Bose-Hubbard model, we develop a method based on a time-dependent generalization of the Gutzwiller ansatz. We calculate the excitations of the homogeneous system both in insulating and superfluid regime, concentrating particularly on those near the superfluid-Mott insulator boundary. Low-lying excitation energies in presence of a static harmonic trap are obtained using this method and compared with the homogeneous case. Further, we explore the dynamics of the center of mass and the breathing mode in response to time-dependent perturbations of the trap.

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The study of ultracold bosonic atoms confined in an optical lattice as a correlated system [1] has been an active area of research in the past few years [2]. It could provide a better understanding of many phenomena driven by strong many-body correlations in a controlled fashion, which is rather difficult to explore in conventional solid state systems. These include the quantum phase transition between the Mott insulating (MI) and the superfluid (SF) phases [3, 4], Luttinger liquid behavior in quasi-one dimensional condensates in the Tonks-Girardeau regime [5], etc. It has been proposed that these systems could be used to simulate various quantum spin models [6], especially in reduced dimensionality and for creation of frustrated lattices to explore the possibility of unconventional quantum phases [7]. It may also be possible to achieve reliable prototypes for quantum computing and information processing [8]. Recent experiments involving dipolar atoms [9] are expected to lead to the realization of new phases of matter such as the supersolid (SS) [10, 11], whose existence is still not unambiguous in solid ⁴He [12].

The MI-SF transition in lattice bosons is controlled by the competition between the interaction among them and their kinetic energy [13]. However, the translational symmetry breaking confining potential, that is present in experiments, would lead to inhomogeneous phases and even phase coexistence for appropriate parameters. There have been various proposals to observe such structures [14]. A clear indication of it will be their excitation spectra, which will be different from their homogeneous counterparts and the way the system behaves under time-dependent perturbations of the trap [15]. Further, the study of the collective modes has become an important experimental tool to analyze correlation properties of ultracold quantum gases in a trap [4, 16]. With this in mind, we systematically explore the excitations of parabolically trapped lattice bosons from deep SF phase to insulating phase. Our method also provides a detailed microscopic understanding of the behavior of the trapped

SF under perturbations which, hitherto, has been studied using the Gross-Pitaevskii equation (GPE) or equivalent hydrodynamic approach [17]. These methods are valid only when the SF fraction is very large; they fail to capture the modified physics both in the homogeneous SF near the MI boundary and in the inhomogeneous phase coexistence regime.

The harmonically trapped alkali atoms with short range interactions in an optical lattice can be modeled by the effective Bose-Hubbard model (BHM) [1, 13]:

$$\hat{H} = -t \sum_{i,\delta} \hat{a}_i^\dagger \hat{a}_{i+\delta} + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) + \frac{m\omega^2}{2} \mathbf{r}_i^2 \hat{n}_i \right]. \quad (1)$$

The three terms represent the lattice kinetic energy, the on-site interaction, and the harmonic trap potential respectively. The operator \hat{a}_i^\dagger creates a boson at site i , $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the boson number operator, \mathbf{r}_i is the distance of the site i from the minimum of the trap potential with frequency ω ; t, U are the nearest-neighbor hopping and the on-site Hubbard interaction respectively, m is the mass of the atoms, and δ represents the nearest neighbors of the site i . This Hamiltonian without any confining potential has been studied extensively using a variety of methods such as the mean field theory [13], quantum Monte-Carlo [18], perturbation series [19] and density matrix renormalization group (DMRG) [20, 21]. In the absence of trap, the ground state is an incompressible MI with an integer number of atoms at every lattice site when the interactions dominate and the particle density is commensurate with the lattice. When the kinetic energy dominates, and in general when the density is incommensurate, a SF ground state is obtained. The low-lying excitations in the MI state are gapped particle-hole excitations. The SF phase has gapless, acoustic, Bogoliubov quasiparticles. For large enough t/U , the excitations can be described by the discrete non-linear Schrödinger (DNLS) equation (the lattice version of the GPE) [17], which becomes progressively inaccurate as

one moves towards the MI-SF boundary [11]. In presence of a trap one encounters an inhomogeneous SF phase and at smaller values of t/U , the renormalized chemical potential gives rise to alternating shells of SF and MI regions. In absence of *numerically exact* calculations, which are not hindered by limited system size or small number of bosons, a (linearized) time dependent variational mean field analysis is an appropriate tool to explore the excitations of these systems; it gives quantitatively correct results [18] in homogeneous case. Hence, we use the variational Gutzwiller mean field approach to study the ground state and use a modified time-dependent Gutzwiller ansatz to study the low-lying excitation energies. In particular, we concentrate on the excitations in the homogeneous phase near the MI-SF boundary, the low-lying spectra in the presence of a static trap as a function of parameters, and the dynamics of the system in response to time-dependent perturbations of trap potential.

We calculate the inhomogeneous ground states of the above model, in general in d dimensions, for a given set of parameters and the chemical potential μ by minimizing $\langle \Psi | \hat{H} - \mu \hat{N} | \Psi \rangle$ with a Gutzwiller wavefunction $|\Psi\rangle = \prod_i \sum_n f_n^{(i)} |n, i\rangle$ with respect to the variational parameters $f_n^{(i)}$, where $|n, i\rangle$ is the Fock state with n particles at site i and $\hat{N} = \sum_i \hat{n}_i$ is the total particle number operator. The excitation energies above the ground state are, then, obtained from the real-space dynamical Gutzwiller approach with the variational parameters $f_n^{(i)}$ being time dependent that was introduced in Ref. [22] and modified for the calculation of excitation spectra in Ref. [11]. Minimization of the effective action $\langle \Psi | i\hbar \frac{\partial}{\partial \tau} - \hat{H} + \mu \hat{N} | \Psi \rangle$ gives the equations of motion for $f_n^{(i)}$:

$$i\hbar \frac{\partial f_n^{(i)}}{\partial \tau} = \left[\frac{U}{2} n_i (n_i - 1) - \mu n_i + \frac{m\omega^2}{2} \mathbf{r}_i^2 n_i \right] f_n^{(i)} - t \sum_{\delta} \left[\phi_{i+\delta}^* \sqrt{n+1} f_{n+1}^{(i)} + \phi_{i+\delta} \sqrt{n} f_{n-1}^{(i)} \right]. \quad (2)$$

Here $\phi_i = \langle \Psi | \hat{a}_i | \Psi \rangle$ is the local condensate (SF) order parameter and τ is time. The oscillation frequencies of the small amplitude fluctuations $\delta f_n^{(i)}(\tau)$ around the ground state $\bar{f}_n^{(i)}$ give the excitation spectrum. Normalization of the wavefunctions, $\sum_n |f_n^{(i)}(\tau)|^2 = 1$, at each site is enforced using a Lagrange multiplier λ_i .

Firstly, we consider the excitations in the homogeneous system without a trap. For the MI phase with n_0 bosons per site, the ground state is defined by $\bar{f}_n^{(i)} = \delta_{n,n_0}$. The resulting linearized equations lead to particle(p) and

hole(h) excitations with dispersions

$$\varepsilon_{p(h)} = \sqrt{\frac{U^2}{4} + \frac{\epsilon_{\mathbf{k}}^2}{4} + \epsilon_{\mathbf{k}} U (n_0 + \frac{1}{2})} \pm \left[U (n_0 - \frac{1}{2}) - \mu + \frac{\epsilon_{\mathbf{k}}}{2} \right], \quad (3)$$

where \pm corresponds to p(h) excitations and $\epsilon_{\mathbf{k}} = -2t \sum_{j=1}^d \cos(k_j)$. This is in agreement with the results obtained from the slave-boson mean-field theory [23] and random-phase approximation [24]. As one approaches the phase boundary from the MI side, the energy gap for p(h) excitations gradually decreases, vanishing at the transition. The phase boundary at which the MI-SF transition occurs is obtained from the condition of vanishing energy-gap, $\varepsilon_{p(h)}(\mathbf{k} = \mathbf{0}) = 0$, and is in agreement with the calculations using second order perturbation theory in t/U [19]. Deep in the SF phase (i.e., when $t \gg U$), and for large SF fraction ($|\phi_i|^2 \sim n_i$), the wavefunction at each site can be represented by coherent states, i.e., $f_n^{(i)} = \phi_i^n e^{-|\phi_i|^2/2} / \sqrt{n!}$ and Eq.(2) reduces to a DNLS equation for the classical field ϕ_i :

$$i\hbar \frac{\partial \phi_i}{\partial \tau} = -t \sum_{\delta} \phi_{i+\delta} + U |\phi_i|^2 \phi_i - \mu \phi_i + \frac{m\omega^2}{2} \mathbf{r}_i^2 \phi_i \quad (4)$$

In the absence of a trap, this gives gapless acoustic mode with sound velocity $c_s = |\phi| a \sqrt{2tU}/\hbar$, where a is the lattice spacing. The MI-SF transition near the Mott lobe at a commensurate density n_0 can be understood *via* a simple three-state variational ansatz at site i : $|\psi_i\rangle = f_1 |n_0 - 1\rangle + f_0 |n_0\rangle + f_2 |n_0 + 1\rangle$. This captures the build-up of number fluctuations [25], and hence the phase coherence as the system makes a transition to the SF phase at a critical coupling $(U/2td)_c = (\sqrt{n_0} + \sqrt{n_0 + 1})^2$. Introducing time-dependent fluctuations in the variational parameters lead to the Bogoliubov spectrum in the SF phase with the sound velocity c_s given by,

$$c_s = t\sqrt{d} \cos \theta \sqrt{(\alpha^2 \cos^2 \theta - 1)/2}, \quad (5)$$

where $\alpha = (\sqrt{n_0} + \sqrt{n_0 + 1})^2 = U/(2td \cos 2\theta)$. Interestingly, at the boundary where $\theta = 0$, the sound velocity is finite, although the SF order parameter ϕ vanishes. This was first pointed out in Ref. [26] with $n_0 \gg 1$ and an effective relativistic GPE has been proposed to capture the dynamics close to the MI phase. For small momenta, the (gapped) amplitude mode [26] in the SF has the dispersion $\omega(\mathbf{k}) = \sqrt{\Delta^2 + c^2 \mathbf{k}^2}$ with $\Delta = td \sin 2\theta \sqrt{\alpha^2 - 1}$ and $c^2 = (t^2 d/8) [9 + (4\alpha^2 - 13) \cos^2 2\theta]$ in d -dimensions. At the boundary, this mode becomes degenerate with the gapless, Bogoliubov mode. However, deep in the SF phase three state variational ansatz is insufficient and we increase the number of Fock states at each site and numerically solve the linearized equations for the fluctuations $\delta f_n^{(i)}$ to obtain the collective mode with momentum k . The dispersion of the lowest acoustic mode in the SF phase is shown in Fig.1 for different coupling

strengths. We compare our result with those obtained from DNLS and find good agreement deep in the SF regime ($|\phi_i|^2 \sim n_i$), whereas DNLS fails near the MI boundary (see Fig.1).

Main advantage of our method is that it is simple and efficient enough to implement in confined geometries and for inhomogeneous systems. Confining traps which are present in experiments can be approximated by a harmonic oscillator potential $V(\mathbf{r}_i) = \frac{1}{2}m\omega^2\mathbf{r}_i^2$. Minimization of free energy gives, in general, inhomogeneous ground state that show coexisting SF and MI phases (with step-like structure) for certain parameters. Compressible edge forms on the boundary of such droplet. Having found the ground state for a given μ , we calculate the low-lying spectrum by solving the system of linearized equations (Eq.(2)). Recently collective excitations of BHM in a 1D harmonic trap have been calculated by exact diagonalization of the Hamiltonian for small system size [27]. However, the complexity of the problem grows exponentially with increasing number of the lattice sites and boson filling fractions. Numerically efficient T-DMRG methods [15, 21] are restricted to 1D systems with short range interactions, whereas our method can be applied to higher dimensions, where the mean field method is expected to work better. In Fig.2 we show

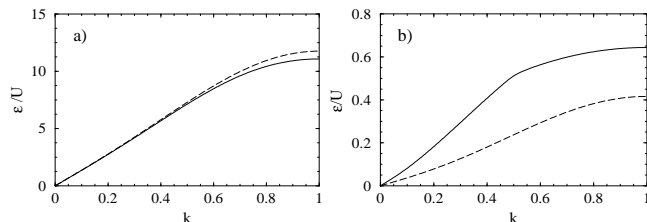


FIG. 1: Excitation spectrum of the uniform BHM with $\mu/U = 0.5$, a) for $t/U = 2$ and b) for $t/U = 0.087$. For comparison dotted lines represent excitation spectrum obtained from DNLS. Momentum k is in units of π/a .

a few low-lying excitations of bosons in a 1D harmonic trap, as a function of t/U for a fixed μ/U . We clearly notice three different regimes by changing the interaction strength t/U . In the deep SF region (i.e., $t/U \gg 1$), excitations are Bogoliubov quasiparticles and their energies asymptotically match with those obtained from DNLS. In this regime the hopping parameter t is equal to the kinetic energy $\hbar^2/(2ma^2)$. For large t/U , the n th excitation branch approaches $\omega\sqrt{n(n+1)}ta^2m$ asymptotically and is in agreement with the hydrodynamic modes of a dilute Bose gas in 1D harmonic trap without a lattice [28]. As the system enters the correlated regime (for smaller t/U), which is close to the phase boundary, the excitation energies start to deviate from those obtained from DNLS and many avoided level crossings occur in the energy spectrum. We notice the clear signature of particle and hole type excitations deep in the MI phase ($t/U \ll 1$). In contrast to the homogeneous BHM, where

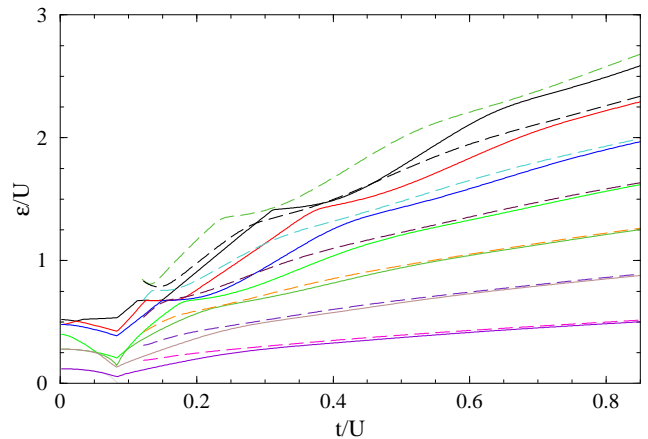


FIG. 2: Few low-lying excitations of the BHM in a trap with $m\omega^2a^2/U = 0.16$ and $\mu/U = 0.6$ (solid lines). For comparison the dotted lines denote the energies obtained from DNLS for the same parameters.

p(h) energies are site-degenerate, in case of harmonically trapped BHM, they split and become site-dependent in the insulating phase. It is easy to understand these p(h) excitation energies in the atomic limit of BHM. For $t = 0$ and $\mu < U$ the system forms a droplet of size $2n_{max}$ with all sites i for $-n_{max} \leq i \leq n_{max}$ filled with one particle per site, where n_{max} being the integer part of $\sqrt{2\mu/(m\omega^2a^2)}$. Thus in presence of the trap, the energy for adding or removing a particle, in general, depends on the site index i , and is given by $E_p = U - \mu + \frac{1}{2}m\omega^2a^2i^2$ and $E_h = \mu - \frac{1}{2}m\omega^2a^2i^2$. At the edge of the trap (at $i = \pm n_{max}$), $E_p \approx U$ and $E_h \approx 0$. Similarly, it costs very little energy to create a particle at the empty site just outside the droplet (i.e., $i = \pm(n_{max} + 1)$). This leads to the formation of the gapless edge at finite t . In SF phase, among the low-lying collective excitations

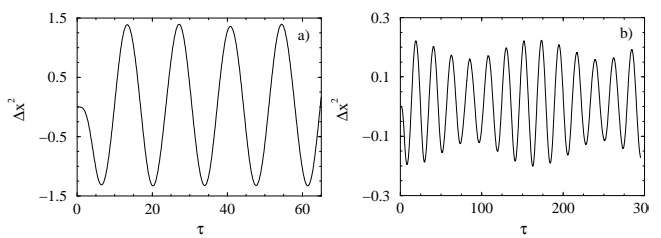


FIG. 3: Time evolution of the breathing mode Δx^2 in a trap with $m\omega^2a^2 = 0.5$, $\mu = 0.8$, a) for $t/U = 0.23$, and b) for $t/U = 0.1$. Length and time are measured in units of a and \hbar/U respectively.

of harmonically trapped lattice bosons, dipole oscillation describing the center of mass motion has the lowest energy. According to Kohn's theorem, dipole excitation energy in a harmonic trap is $\hbar\omega$ that is independent of two-body interaction [17]. In case of BHM the dipole excitation energy deviates from this universal value due to the presence of the optical lattice. For large system size and deep in the SF phase we find that it approaches

$\sqrt{2tm\omega}a$, in agreement with Kohn's theorem. In experiments, dipole mode can be excited by slightly shifting the atomic cloud from the center of the trap by imposing a perturbation of the form $V_{pert} \sim \sum_i x_i \hat{n}_i$.

Having studied the spectra in the presence of a static trap, we now concentrate on the effect of time-dependent perturbations of the trap on the dynamics of BHM by solving the full time-dependent Gutzwiller equation. As an example, we focus on an experimentally relevant collective mode of 1D confined system, the breathing mode, where the center of mass of the atomic cloud remains fixed but its size oscillates. For harmonically trapped dilute Bose gas in quasi 1D regime, the frequency of this oscillations is $\sqrt{3}\omega$ [28]. Experimental study of this mode has become an important tool for the investigation of the correlation properties of quasi 1D quantum gases, particularly when 1D Bose gas enters the strongly correlated fermionized regime [28]. We study the breathing mode as a linear response to a perturbing potential of the form $V_{pert} \sim \sum_i x_i^2 \hat{n}_i$. Oscillation frequencies of both dipole and breathing modes obtained from the full dynamics agree with those obtained from linearized time dependent method. In Fig.3, time evolutions of the collective coordinate $\Delta x^2 = \sum_i [\langle x_i^2(\tau) \rangle - \langle x_i^2(0) \rangle]$ are shown for two different values of t/U , under the same perturbation strength. We observe that the response of the system becomes smaller as it approaches the insulating regime. The MI phase hardly responds to perturbations due to the energy gap in the spectrum [29]. In the SF phase with small t/U (close to the MI boundary), the breathing mode oscillations show beats instead of a single frequency. As noted earlier, in this regime excitation energies are very close to each other and many avoided level crossings occur (see Fig. 2). Due to this reason mode coupling takes place leading to beats in the dynamics of the collective modes.

In conclusion, we develop a new time-dependent variational method to obtain the spectra of correlated lattice bosons in an (arbitrary) confining potential. In the homogeneous phase, we find that, at commensurate filling and at the SF-MI boundary, the sound velocity does not vanish even though the SF order parameter vanishes. Low-lying excitations of BHM in a harmonic trap are obtained, which validates the GPE approach asymptotically, while deviating significantly in the correlated regime. The dynamics of the collective coordinates under time-dependent perturbations reveals decrease in their amplitudes as well as appearance of beats in the strongly correlated regime. These results are relevant to the experimental observation of coexisting MI-SF phases and measurements of their dynamical properties.

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